Albany: A Trilinos-based code for Ice Sheet Simulations and other Applications

Andy Salinger (SNL)

Irina K. Tezaur, Mauro Perego, Ray Tuminaro & Steve Price (LANL)

Roger Pawlowski, Irina Demeshko, Eric Phipps

Deployment and Application of Technologies provided by the FASTMath Institute

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Support from:

Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

What is the Albany Code?

- Finite Element Code
  - Implicit
  - Unstructured Grid
  - Massively Parallel
- Demonstrates Component-Based Code design
  - Libraries
  - Abstract Interfaces
  - Pretty good Software Engineering (for CSE)
- Embedded Analysis Capabilities
  - Automatic Differentiation;
  - Sensitivity Analysis; Stability Analysis; Optimization; UQ

Who is the targeted Albany customer base?

➢ **CSE.**

Albany is built on Trilinos:
Leveraging code, software, and expertise

Analysis Tools *(black-box)*
- Optimization
- UQ (sampling)
- Parameter Studies
- Bayesian Calibration

DAKOTA

Software Quality
- Version Control
- Regression Testing
- Configure / Build System
- Test Harness / Dashboard
- Continuous Integration

Albany

Trilinos

Analysis Tools *(embedded)*
- Nonlinear Solver
- Time Integration
- Continuation
- Sensitivity Analysis
- Stability Analysis
- Optimization
- UQ Solver

Utilities
- Input File Parser
- Parameter List
- Memory Management

Discretizations
- Discretization Library
- Field Manager

Linear Algebra
- Data Structures
- Iterative Solvers
- Direct Solvers
- EigenSolver
- Preconditioners
- Multi-Level Methods

Mesh Tools
- Mesh Database
- Mesh I/O
- PARTITIONING
- Load Balancing
- Adaptivity

Derivative Tools
- Derivatives
- Sensitivities
- Adjoints
- UQ Propagation

NextGen Architectures
- Data Structures
- Programming Model

Laboratories

SciDAC Institutes and ASCR Support Several Key Components

Analysis Tools (*black-box*)
- Optimization
- UQ (sampling)
- Parameter Studies
- Bayesian Calibration

QUEST — QUANTIFICATION OF UNCERTAINTY IN EXTREME SCALE COMPUTATIONS

IDEAS productivity

Software Quality
- Version Control
- Regression Testing
- Configure / Build System
- Test Harness / Dashboard
- Continuous Integration

Analysis Tools (*embedded*)
- Nonlinear Solver
- Time Integration
- Continuation
- Sensitivity Analysis
- Stability Analysis
- Optimization
- UQ Solver

FASTMATH

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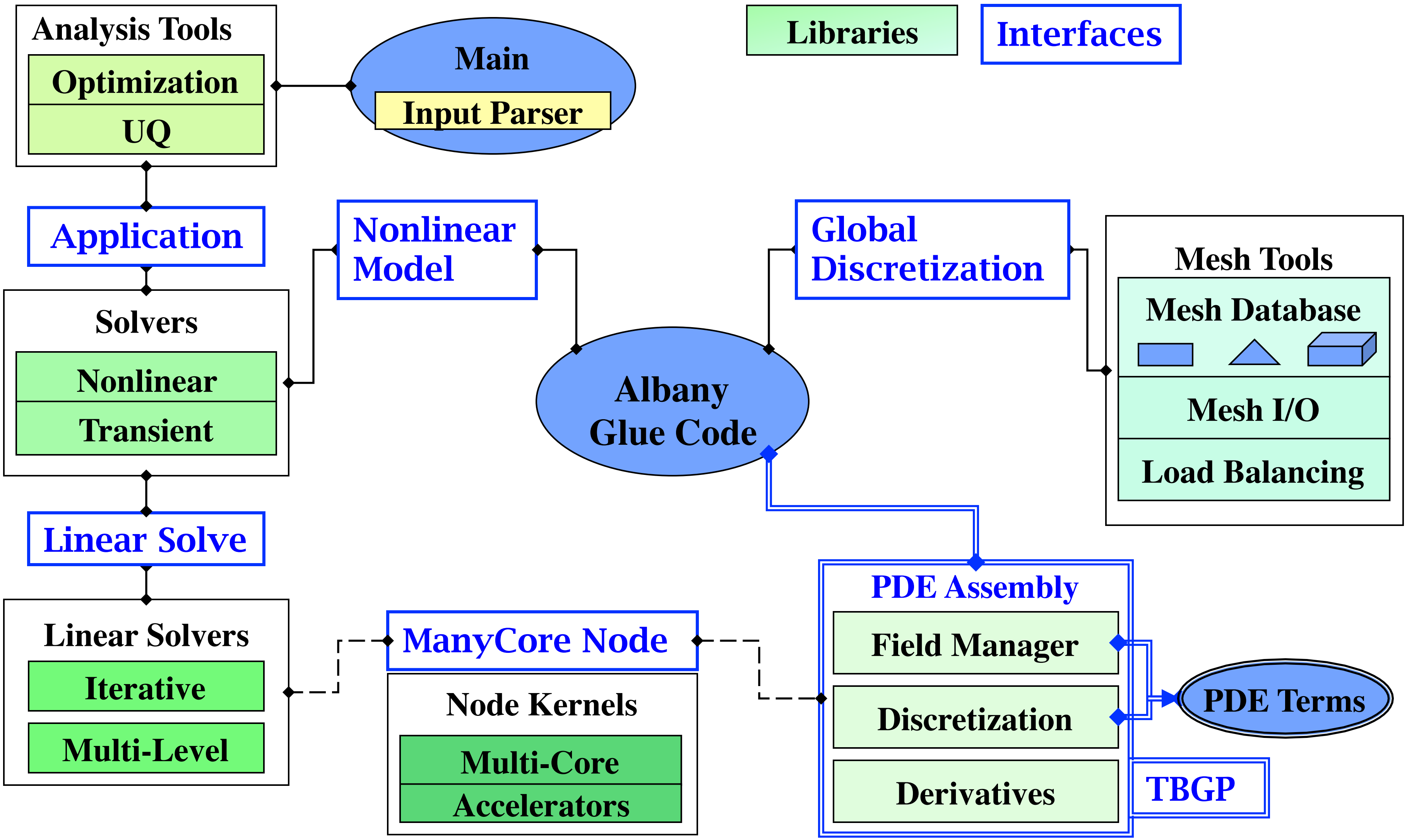
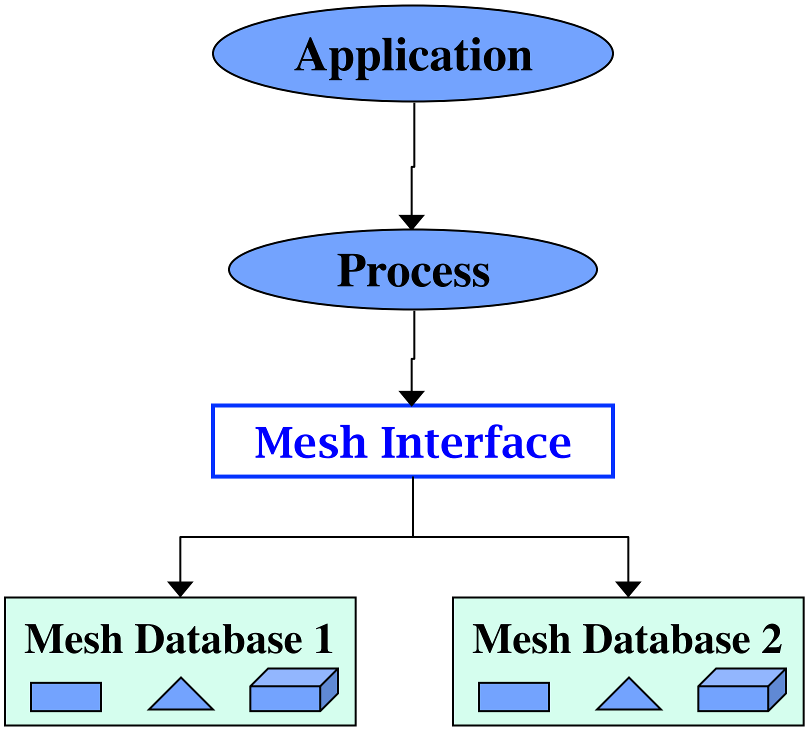
Laboratories

Well-Designed Interfaces make Component-Based Code Design a Scalable Endeavor

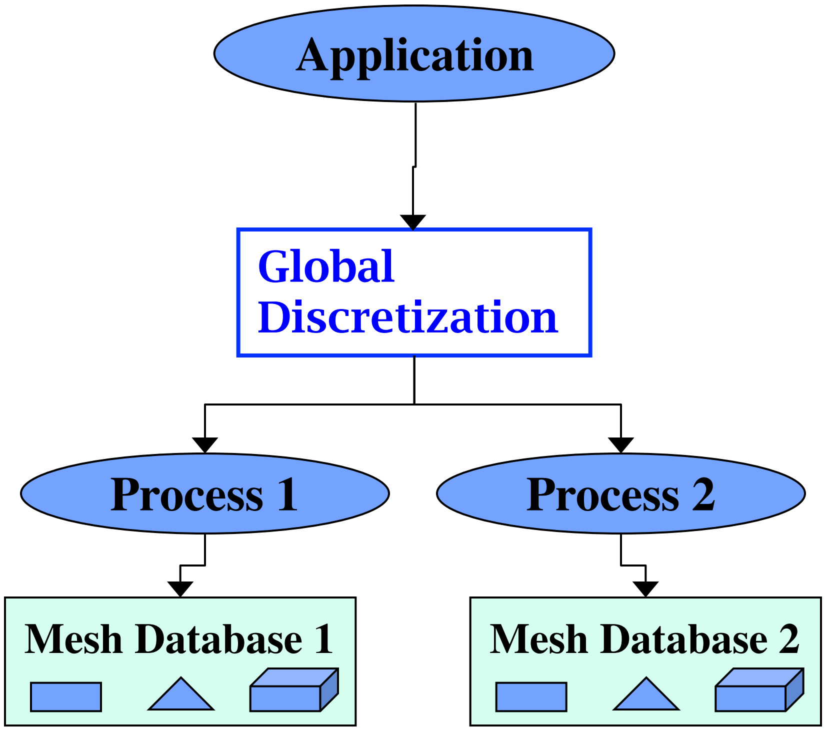


Interface Design: *What does Albany use for a Mesh Interface?*

1. Mesh Interface Design



2. Global Discretization Design



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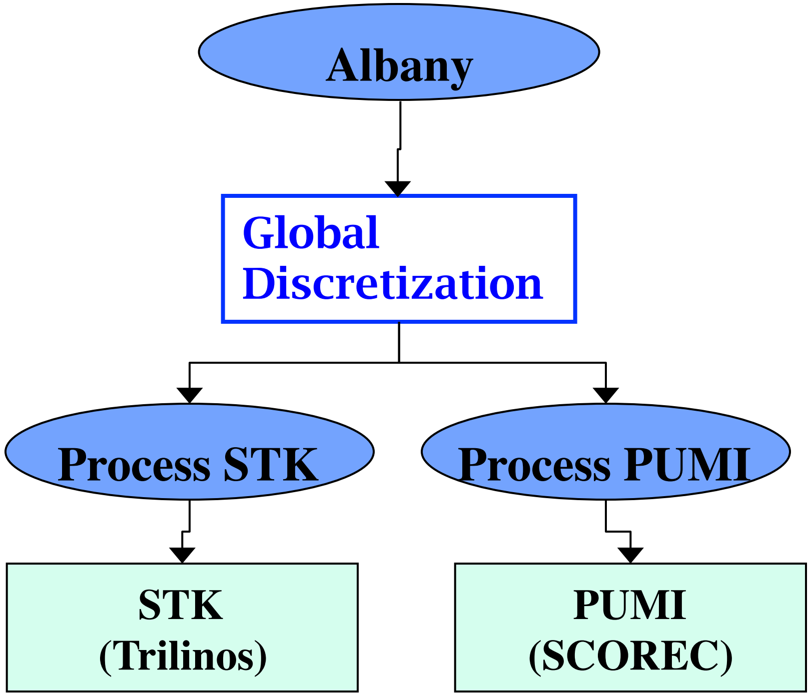
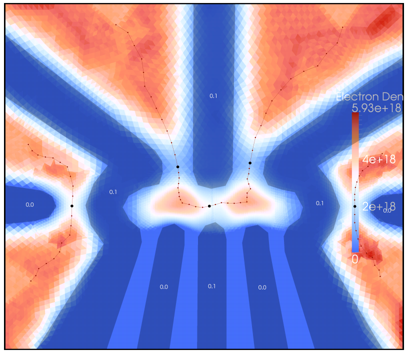
Interface Design: Design of Global Discretization Interface

Global Discretization:
- getCoordinates()
- getConnectivity()
- getOwnedUnknownMap()
- getOverlapUnknownMap()
- getJacobianGraph()
- getSolution()
- writeSolution(x)

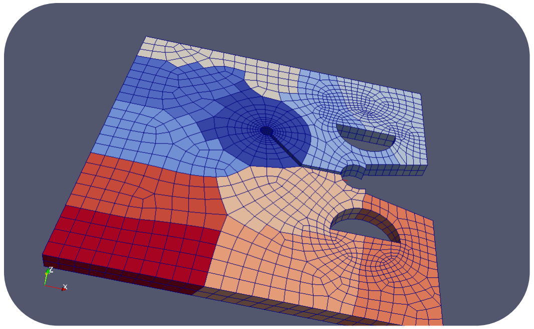
Global Discretization Design



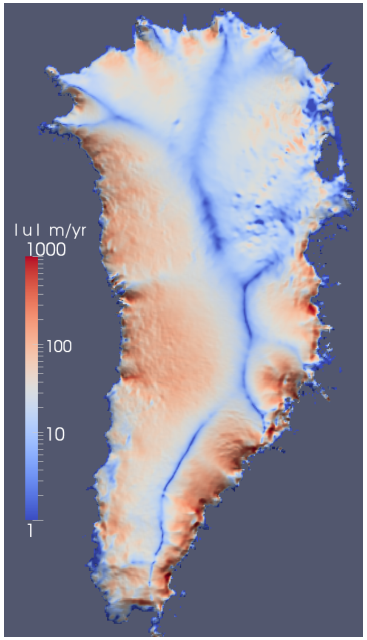
Albany is the Vehicle for Several Application and Algorithm Projects



QCAD:
- Quantum Dot Design



LCM:
- Large Deformation Mechanics
- Failure/Fracture
- Multi-Scale Modeling



FELIX:
- Ice Sheets

Algorithm efforts developed/tested in Albany

1. Mesh Adaptive Loop   Following Talk -- Granzow
2. Embedded UQ
3. Adjoint Gradients with AD
4. Reduced Order Modeling
5. Topological Optimization
6. Performance-Portable Finite Element Assembly

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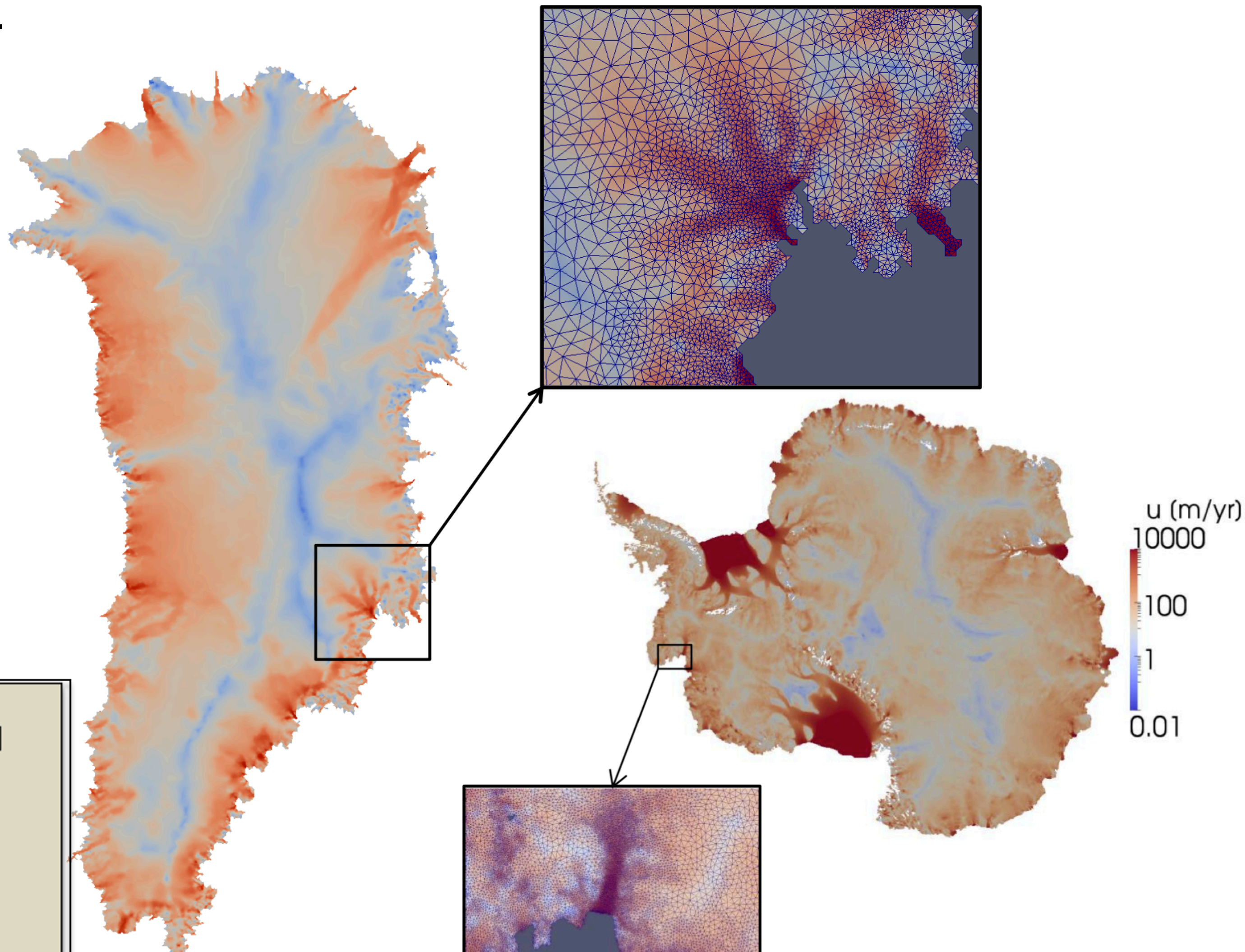
Albany/FELIX code is Supported by PISCEES SciDAC

- Unstructured Grid
- 3D, 2 PDEs
- Steady
- Inversion
- Calibration
- Links under ACME Earth System Model

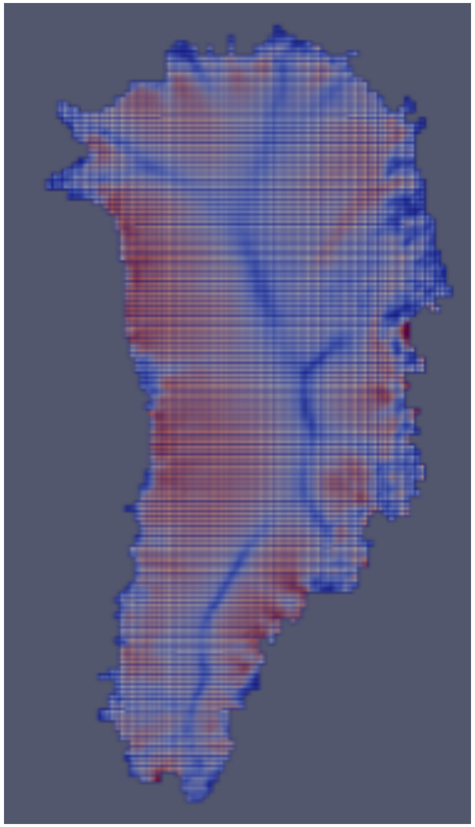


Nonlinear Stokes' Model for Ice Sheet Stresses

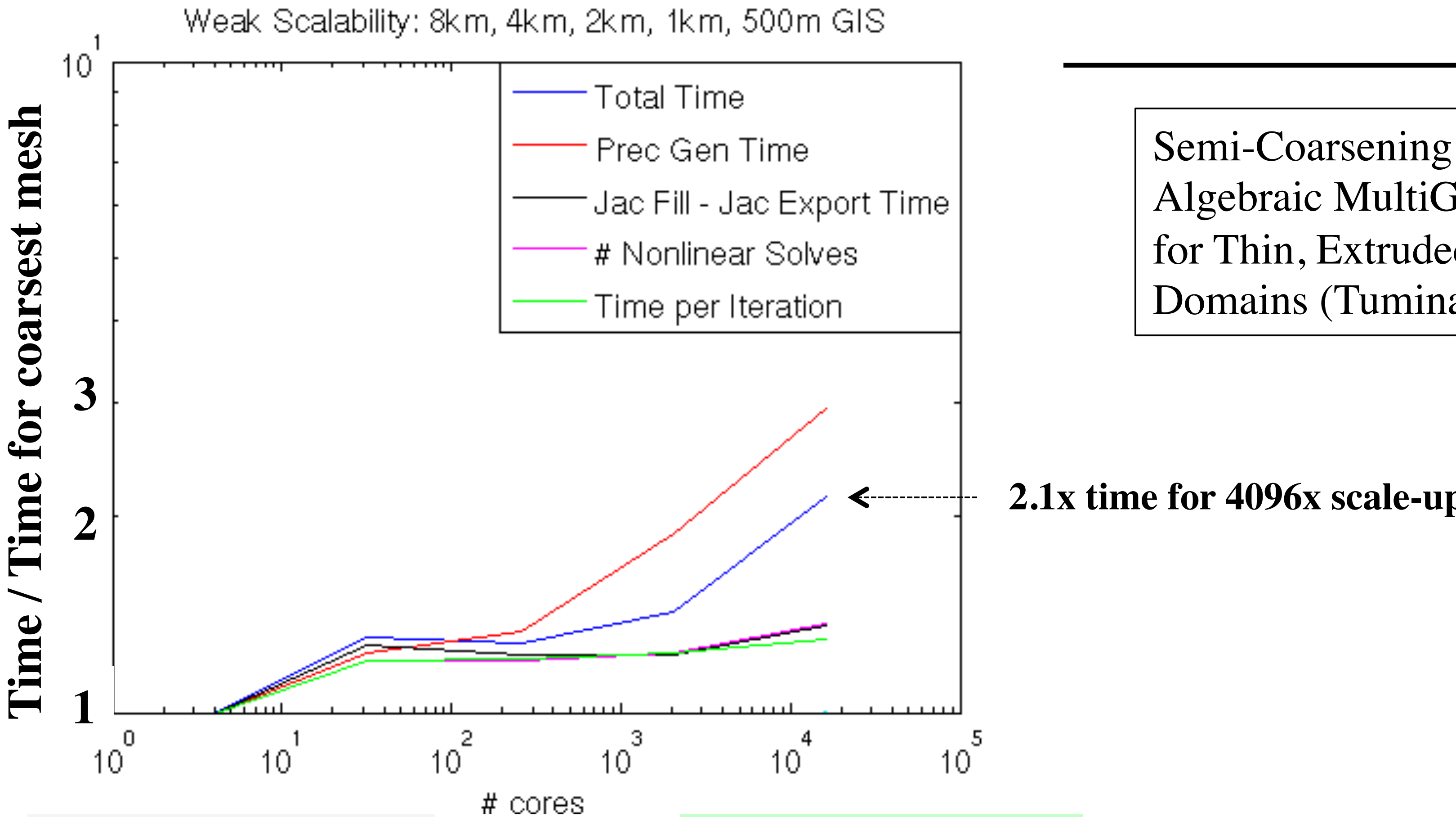
$$-\nabla \cdot (2\mu\dot{\epsilon}_1) = -\rho g \frac{\partial s}{\partial x}$$
$$-\nabla \cdot (2\mu\dot{\epsilon}_2) = -\rho g \frac{\partial s}{\partial y}$$

Albany/FELIX: Verification and Mesh Convergence

Horiz. res.\vert. layers	5	10	20	40	80
8km	2.0e-1				
4km	9.0e-2	7.8e-2			
2km	4.6e-2	2.4e-2	2.3e-2		
1km	3.8e-2	8.9e-3	5.5e-3	5.1e-3	
500m	3.7e-2	6.7e-3	1.7e-3	3.9e-4	8.1e-5



Albany/FELIX: Weak Scalability



Semi-Coarsening Algebraic MultiGrid for Thin, Extruded 3D Domains (Tuminaro)

4 cores
334K dofs
8 km Greenland,
5 vertical layers

→

16,384 cores
1.12B dofs
0.5 km Greenland,
80 vertical layers

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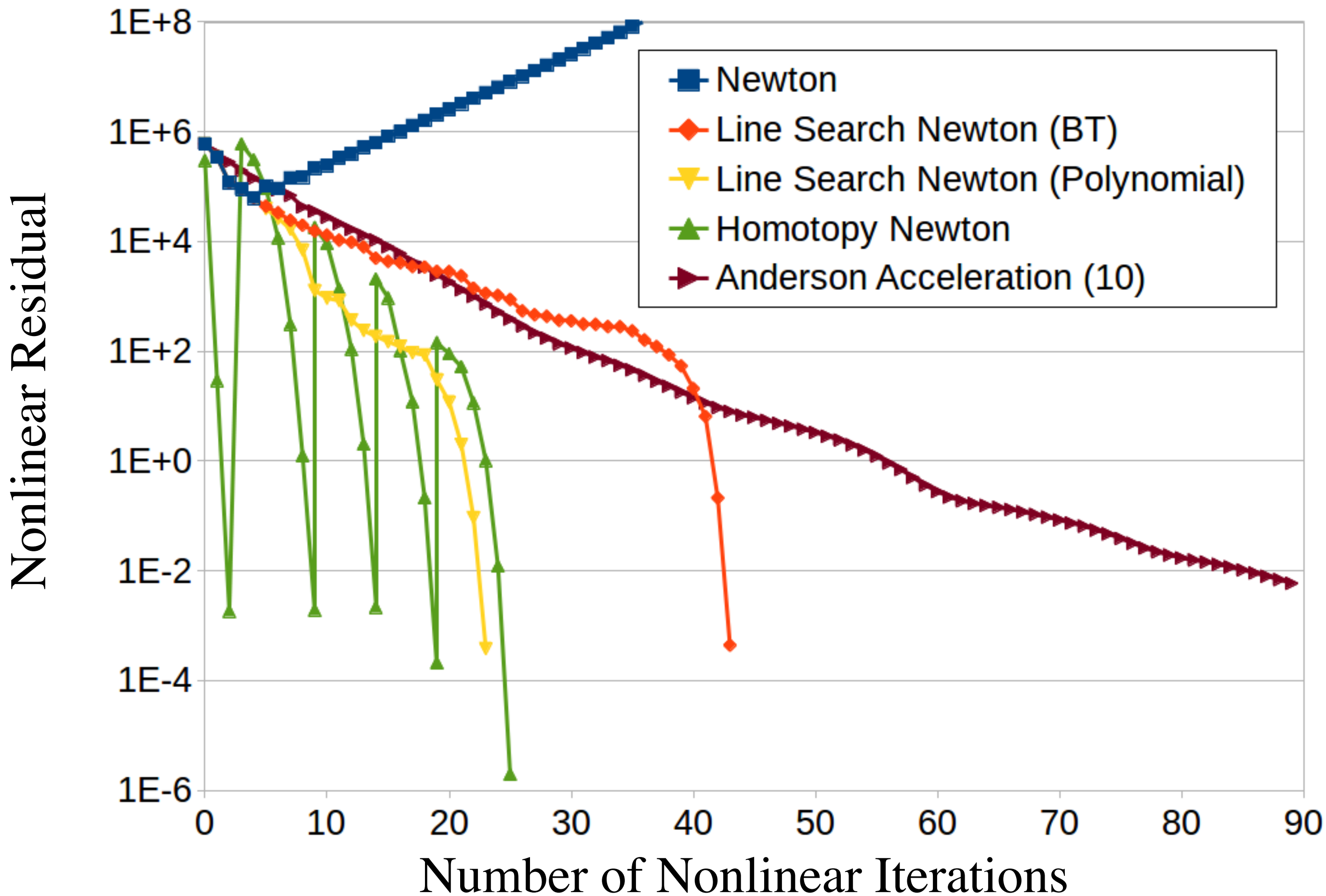
Nonlinear Solvers Robustness is Critical:
Land Ice Solver Inside of Climate Model

$$\mu = \frac{1}{2} A^{-\frac{1}{n}} \left(\frac{1}{2} \sum_{ij} \dot{\epsilon}_{ij}^2 + \gamma \right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)}$$

$\gamma = 10^{-10}$



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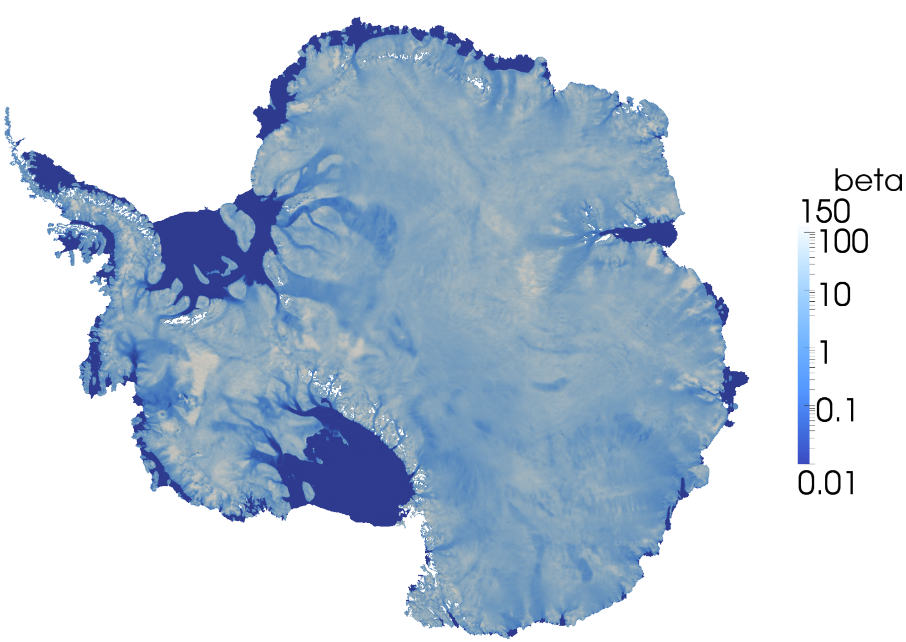
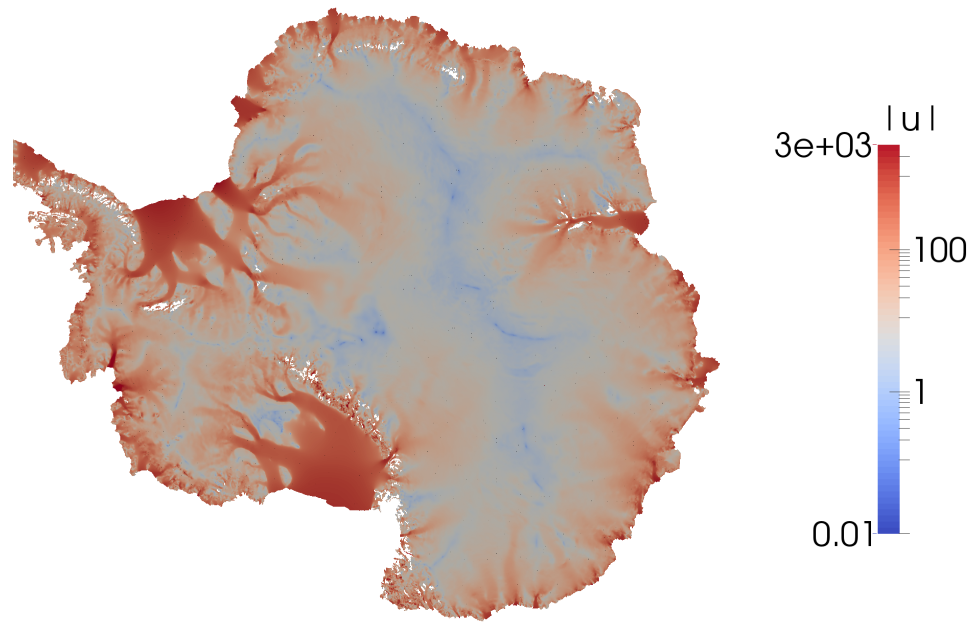
Ice Sheet Initialization: Invert for Basal Sliding Coefficient to Match Observations

Objective functional: $\mathcal{J}(\mathbf{u}(\beta),\ \beta) = \int_\Sigma \frac{1}{\sigma_u^2} |\mathbf{u} - \mathbf{u}^{obs}|^2 \, ds + \ \alpha \int_\Sigma |\nabla \beta|^2 \, ds$





Inverted for 700K Parameters

Developed General Purpose Code for Adjoint-Based Gradients using Automatic Differentiation (Perego, Phipps)

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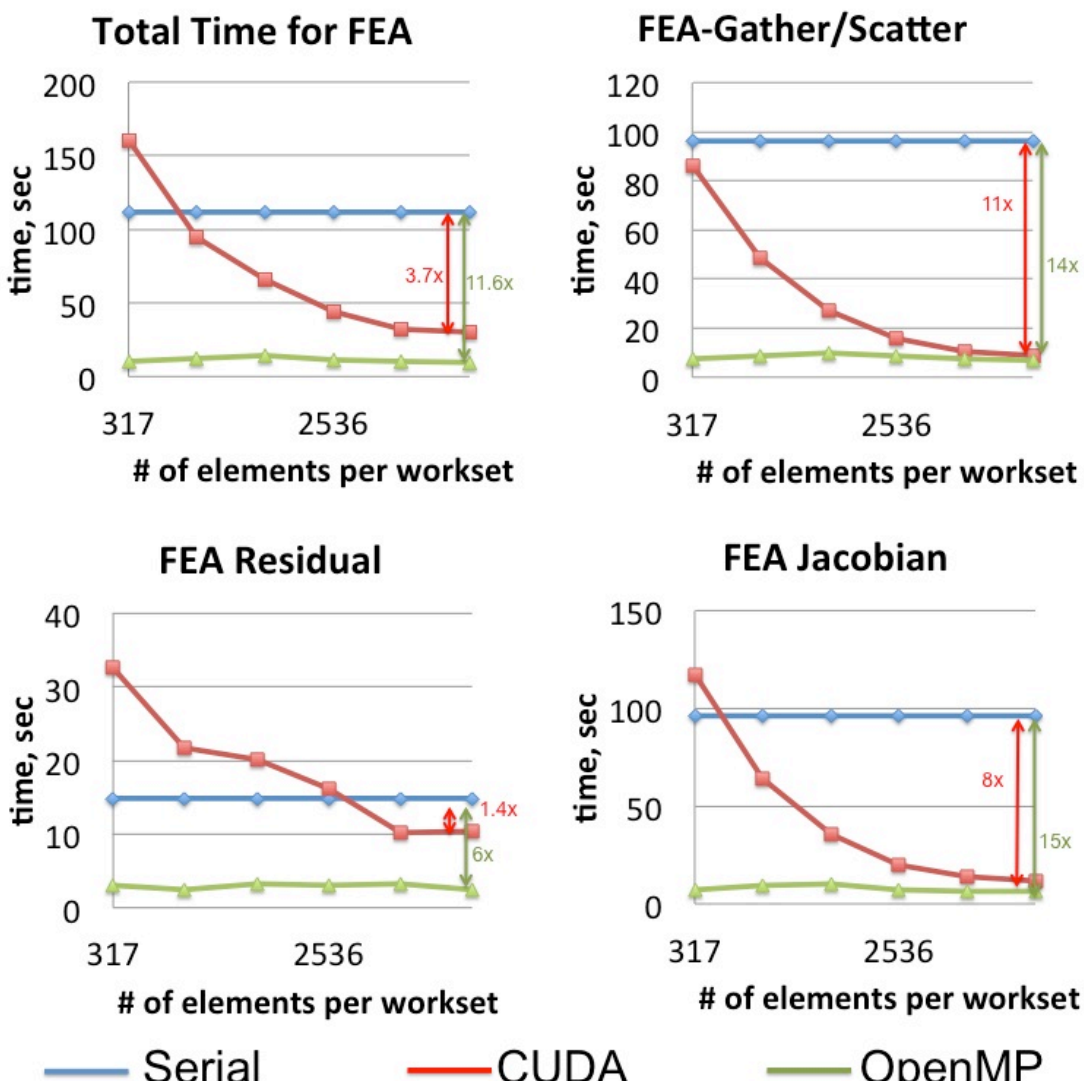
Finite Element Assembly Refactored to use Kokkos Programming Model



Conclusion:
The SciDAC Vision Can be Successful

Using many libraries requires good software design and practices.

Albany/FELIX code leverages code (expertise):

- Mulri-Level Preconditioning code and research (Tuminaro)
- Nonlinear Solver code and research (Pawlowski)
- Adjoint-Based Inversion (Perego, Phipps, Ridzal, Kouri)
- Performance-Portable FE Assembly (Demeshko)

✦Adaptivity

✦Embedded UQ

✦Bayesian Calibration

Acknowledgements: FASTMath, PISCEES, ATDM, OLCF

~30 other Trilinos/Albany/Dakota developers

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